USING THE DELETE-A-GROUP JACKKNIFE VARIANCE ESTIMATOR IN PRACTICE

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KEY WORDS: Calibrated weight; Multi-phase sampling; Poisson sampling; Ratio-adjusted weight; Replicate weight; Restricted regression; Systematic probability sampling.

1. INTRODUCTION

This paper addresses the construction of delete-a-group jackknife variance estimators for a variety of estimation strategies (an estimation strategy is a sampling design paired with an estimator). Relevant theoretical comments will be made where appropriate, but most proofs are left for the appendices of a companion document: "Using the Delete-a-Group Jackknife Variance Estimator in NASS Surveys"(Kott 1998).

The sampling designs to which the delete-a-group jackknife can be applied may have any number of phases. At each phase, one of the following selection schemes is assumed to be used:

1) stratified simple random sampling without replacement,

2) systematic probability sampling (usually called systematic probability proportional to size sampling; here we want to de-emphasize the "size" measure),

3) the converse of systematic probability sampling (what remains in a frame after a systematic probability sample has been removed), or

4) Poisson sampling (in which each element is given its own selection probability, and the sampling of one element has no impact on whether another gets selected).

All stratum samples are assumed to be large (contain at least five sampling units). Violation of this assumption in the first-phase of sampling can cause the delete-a-group jackknife to be biased upward. This is shown in the Appendix.

"Calibration" is a general term for a sampling-weight adjustment that forces the estimates of certain item totals based on the sample at one phase of sampling to equal the same totals based on a previous phase or frame (control) data.

Ratio adjustments, the most common form of calibration, were used repeatedly by the National Agricultural Statistics Service (NASS) in the 1996 Agricultural Resource Management Study (ARMS). Restricted regression, another population form of calibration, was used in both the 1997 Minnesota pilot Quarterly Agriculture Survey (QAS) and the second phase of the 1996 Vegetable Chemical Use Survey (VCUS). Only these forms of calibration are discussed in the text.

The concise term "variance estimation" will be used throughout the text in place of the more cumbersome "mean squared error estimation." It should be understood, however, when the delete-a-group jackknife is a good estimator for the variance of a randomization-consistent estimator, it is also a good estimator for its mean squared error.

For our purposes, the term "nearly unbiased" will mean that the bias of the estimator in question is an ignorably small fraction of its mean squared error. The term "biased" will be used to mean "not (necessarily) nearly unbiased."

When first-phase stratum sample sizes are large, the delete-a-group jackknife is appropriate (has only a small potential for bias) whenever the conventional, randomization-based, delete-one jackknife is. Kott and Stukel (1997) have extended the use of the delete-one jackknife to two-phase estimators with calibration in the second phase. This paper relies heavily on their results. Here, however, systematic probability can be used in the second design phase, even though Kott and Stukel only treated strategies featuring stratified simple random sampling in the second phase.

Section II provides on overview of why one would use a delete-a-group jackknife, while Section III provides on overview of how. Section IV focuses on paticular practical cases (stratified simple random sampling; calibration of a second-phase sample to a vector of first-phase totals using restricted regression or ratio adjustment). Section V addresses finite population correction in its simplest context: a single-phase Poisson sample. An appendix provides some theoretical support for the use of the delete-a-group jackknife variance estimator.

II. WHY USE THE DELETE-A-GROUP JACKKNIFE?

The delete-a-group jackknife is simple to compute once appropriate replicate weights are constructed. The so-called "linearization" methods traditionally used by NASS for estimating variances can be very cumbersome when applied to estimators based on multi-phase samples. Estimators using calibrated weights derived from restricted regression pose even greater practical problems for linearization variance methods (a multivariate regression coefficient would need to be estimated for every item of interest).

The advantage of the delete-a-group jackknife over the traditional, delete-one-primary-sampling-unit-at-a-time jackknife (see Rust 1985) is that the number of needed replicate weights per sample record is kept manageable. A common practice for handling this problem with the delete-one jackknife is to group primary sampling units (PSU's) into variance PSU's. This practice reduces the number of replicate weights needed per record – there is one for every variance PSU. There is a problem when one needs to produce national and state-level estimates from the same survey. At least 15 replicate weights per record would be needed to compute variances for each state-level estimator. This would result in national variance estimates employing several hundred replicate weights per record.

III. COMPUTING A DELETE-A-GROUP JACKKNIFE: AN OVERVIEW

Suppose we have a sampling design with any number of phases and a randomization-consistent estimator, t, we wish to apply to the resultant sample. To compute a delete-a-group jackknife variance estimator for t, we first divide the first-phase sample – both respondents and non-respondents – into R (jackknife) groups. Currently, R is 15 in NASS applications. Consequently, we will assume R = 15 in what follows. By setting R at 15, we lengthen the traditional, normality-based 95% confidence interval by ten percent. To see why this is so, observe that the ratio of the t-value at 0.975 for a Student's t distribution with 14 degrees of freedom and the normal z-value at 0.975 is approximately 1.1.

Suppose we have a survey which may have multiple phases. Let F be the sample selected at the first phase of the sampling process. The first-phase sample units may be composed of distinct elements (e.g., farms) or it may consist of clusters of elements (e.g., area segments). Many survey designs feature a single phase of sample selection.

The delete-a-group jackknife begins by dividing the first-phase sample F, into 15 groups. This can be done as follows: order F in an appropriate manner (discussed below); select the first, sixteenth, thirty-first, ... units for the first group; select the second, seventeenth, thirty-second, ..., units for the second group; continue until all 15 groups are created. Unless the number of units in F is divisible by 15 (which is unlikely), the groups will not all be of the same size.

Ordering in an "appropriate manner" depends on the context. If F was drawn using stratified random sampling, then order the sample so that units in the same stratum are listed together (i.e., contiguously). If samples were drawn using Poisson sampling, order the sample units randomly.

Let S denote the final respondent sample used to compute t, and let w_i denote the sampling weight for element i in S. The elements in S may be the same as the sample units in F or they may be a subsample of those units. The elements in S may also have a different nature than the original sample units in F; for example, they may be farms as opposed to area segments or fields as opposed to farms. In all such cases, however, each element in S must be contained within an original sample unit in F in a clearly defined way. Let e_i be the original sampling weight of the unit containing i (which may be i itself); that is, e_i is the inverse of the unit's first-phase probability of selection.

Let S_r denote that part of the final sample originating in first-phase sample units assigned to group r. The *jackknife replicate* $S_{(r)}$ is the whole final sample S with S_r removed. We similarly define $F_{(r)}$ as the set of first-phase sample units not in r.

We need to create 15 sets of *replicate weights* $\{w_{i(r)}\}$, one for each r, in the following manner: $w_{i(r)} = 0$ for all elements in S_r; for other elements, $w_{i(r)}$ will be close to $(15/14)w_i$ but adjusted to satisfy calibration constraints similar to those satisfied by w_i (exactly how to do this in a number of situations is the subject matter of the following section). *Observe that a $w_{i(r)}$-value has been assigned to every element in S including those in S_r.*

Now t is an estimate based on the sample S calculated using the set of weights, $\{w_i\}$. Let $t_{(r)}$ be the same estimate but with the member of $\{w_{i(r)}\}$ replacing $\{w_i\}$.

The delete-a-group jackknife variance estimator for t is

$$v_J = (14/15) \sum^{15} (t_{(r)} - t)^2. \quad (1)$$

IV. PARTICULAR CASES

In this section, we see how the delete-a-group jackknife can be fruitfully applied in a number of estimation strategies where fpc may be ignored; that is, when the first-phase selection probabilities are all small (say less than or equal to 1/5).

One sampling design *not* discussed in detail here is stratified multi-*stage* sampling, in which subsampling within each primary (first-stage) sampling unit is conducted independently of subsampling in other primary sampling units. When the first stage of sampling has ignorably small selection probabilities, the conventional variance estimator for a stratified multi-stage sample looks exactly like that for a stratified single-stage cluster sample with estimated totals for primary sampling units used in place of actual values. As a result, when a delete-a-group jackknife is appropriate for an estimator based on a stratified single-stage sample, it is appropriate for an estimator based on a stratified multi-stage sample.

Stratified Simple Random Sampling

Suppose we have a single-phase stratified simple random sample without any nonresponse (handling nonresponse will be discussed later). The original and final sampling weight for a unit i in stratum h is $e_i = w_i = N_h/n_h$, where N_h is the population size of stratum h and n_h is its sample size.

Let us now consider the r'th set of replicate weights. For a unit i in $S_{(r)}$ and stratum h, $e_{i(r)} = (15/14)N_h/n_h$. By contrast, the appropriate final r'th replicate weight for unit i *recognizes the calibration equations inherent in the direct expansion estimator*: $N_h = \sum_{j \in S(r) \cap h} w_{j(r)}$ for all h. As a result, the r'th replicate weight is $w_{i(r)} = N_h/n_{h(r)} = (n_h/n_{h(r)})e_i$, where $n_{h(r)}$ is the number of sample units in both $S_{(r)}$ and h. Observe that $e_{i(r)} = w_{i(r)}$ only when n_h is divisible by 15.

Stratified Systematic Probability Sampling

Suppose we have a single-phase, stratified systematic probability sample. The original and final sampling weight for a unit i in stratum h is $e_i = w_i = M_h/(n_h m_i)$, where m_i is the measure of size of unit i in stratum h, M_h is the sum of the m_j across all units in stratum h, and n_h is the stratum sample size.

Analogous to the simple random sampling case, the appropriate final r'th replicate weight for element i recognizes the calibration equations inherent in the Horvitz-Thompson expansion estimator (i.e., $M_h = \sum_{j \in S(r) \cap h} w_{j(r)} m_j$ for all h). It is $w_{i(r)} = (n_h/n_{h(r)})e_i$, where $n_{h(r)}$ is the number of sample units in both $S_{(r)}$ and h.

Stratified simple random sampling can be viewed as equivalent to a special case of systematic probability sampling from randomly-order lists (one in which m_i is constant within strata). The appendix provides some theoretical justification for using the delete-a-group jackknife as described above with a stratified, single-phase systematic probability sampling design under certain conditions. One of those conditions is that the systematic samples be drawn from *randomly*-ordered lists. Variance estimation can be problematic when systematic samples are drawn from *purposefully*-ordered lists.

Purposefully-ordered lists can reduce the variance in estimators based on systematic samples. Unfortunately, the reduction in variance due to a well-designed ordering usually can not be measured in an effective manner.

Restricted Regression (A Form of Calibration)

Suppose, for exposition purposes, we have a sampling design with two phases. Suppose further that the second phase sample is calibrated to a row vector of totals, η, based on estimates from the first-phase sample or determined from the frame itself.

Let f_j be the weight for element j after the first phase of sampling, and let p_j be the element's selection probability in the second sampling phase. In the absence of non-response (again, nonresponse will be dealt with later) in the second sampling phase, a general form of the calibrated weight for j under restricted regression is

$$w_j = f_j/p_j + (\eta^* - \sum_{i \in S^*} [f_i/p_i]\mathbf{x}_i) (\sum_{i \in S^*} [f_i/p_i]\mathbf{x}_i'\mathbf{x}_i)^{-1} [f_j/p_j]\mathbf{x}_j' \quad (2)$$

for $i \in S^*$, and a predetermined value otherwise (chosen so that w_j is not too small or too far from f_j/p_j), where S is the second-phase sample, S* a subset containing almost all the elements of S, $\mathbf{x}_i$ is a row vector of covariates whose sum across all elements in the population is either η or has been previously estimated to be η – that is, $\eta = \sum_F f_i\mathbf{x}_i$, where F denotes the elements in the first-phase sample; finally, η^* =

$\eta - \sum_{S-S*} w_i \mathbf{x}_i$.

Let $f_{j(r)}$ be the r'th jackknife replicate weight for unit j after the first sampling phase. The r'th jackknife replicate weight for element j is 0 when $j \in S_r$; otherwise, it is

$$w_{j(r)} = w_j[f_{j(r)}/f_j] + (\eta_{(r)} - \sum_{i\in S(r)} w_i[f_{i(r)}/f_i]\mathbf{x}_i) (\sum_{i\in S(r)} w_i[f_{i(r)}/f_i]\mathbf{x}_i'\mathbf{x}_i)^{-1} w_j [f_{j(r)}/f_j]\mathbf{x}_j', \quad (3)$$

where $\eta_{(r)} = \eta$ when η has been determined from frame; $\eta_{(r)} = \sum_F f_{i(r)}\mathbf{x}_i$ when η has been estimated from the first-phase sample.

Equation (3) is *not* the standard way to construct jackknife replicate weights. The expression $w_k[f_{k(r)}/f_k]$ has been used in place of the more common $f_{k(r)}/p_k$, with which it is nearly equal (because $w_k \approx f_k/p_k$). Equation (3)'s strength is that it forces the replicate weights (for elements not in group r) to be fairly close to the associated calibrated weights. This appears to reduce the upward bias that unexpected differences between the two can cause. It should be noted that any such upward bias is small; in fact, it is asymptotically ignorable. We live, however, in a finite world.

Restricted-regression as described above can be done at any phase of sampling. At the t'th phase, f_i in equation (2) becomes the weight for element i at the t-1'th phase and p_i the element's conditional selection probability at the t'th phase. For a single-phase restricted-regression estimator, we can set all $p_i = 1$ in equation (2).

When the phase of sampling calibrated in this manner contains more than a single stratum, the jackknife can have an upward bias. In addition, for a single-phase Poisson sample, $\mathbf{x}_i\boldsymbol{\lambda} = 1$ must hold for some $\boldsymbol{\lambda}$. See Kott (1998).

Ratio-Adjusted Weights (Another Form of Calibration)

Consider, again, a two-phase sample with f_i and p_i as above. A very common form of calibration occurs when a vector of covariates for element i, $\mathbf{x}_i$, is defined in such a way that only one component of the vector is non-zero for each i. That is to say, the elements are categorized into G mutually exclusive calibration (or ratio-adjustment) groups, and $x_{ig} > 0$ only when element i is in group g; otherwise, $x_{ig} = 0$.

Under that structure, a ratio-adjusted weight for an element j in group g is

$$w_j = \eta_g (\sum_{i\in S} [f_i/p_i]x_{ig})^{-1}[f_j/p_j], \quad (4)$$

and $\eta = (\eta_1, ..., \eta_G)$. Similarly, the corresponding replicate weight is 0 for $j \in S_r$, and

$$w_{j(r)} = \eta_{g(r)} (\sum_{i\in S(r)} f_{i(r)}/p_i]x_{ig})^{-1}[f_{j(r)}/p_j] \quad (5)$$

otherwise, where $\eta_{(r)} = (\eta_{1(r)}, ..., \eta_{G(r)})$.

If the second-phase sample is stratified, and more than one of these strata are contained within a calibration group, then the jackknife can have an upward bias.

Extensions of these results to estimation strategies with t > 2 phases are straight-forward; the f_i in equation (4) and $f_{i(r)}$ in equation (5) become the weight and replicate weight at the t-1'th phase. For a single-phase sample, we can set all the p_i equal to 1 in both equations (4) and (5).

V. SINGLE-PHASE POISSON SAMPLING AND FINITE POPULATION CORRECTION

In this section, we restrict our attention – at first – to a single-phase Poisson sample of elements. Let π_j be the selection probability of element j. We assume there is no nonresponse.

The versions of the delete-a-group jackknife developed in this section *will* contain finite population corrections. The versions are different for an estimator of a total and the estimator of a ratio. This is a reflection of the fact that *a simple formula like equation (1) does NOT work for all smooth transformations of calibrated expansion estimators when finite population correction is an issue* (note: a "smooth" transformation has first, second, and third derivatives; most statistics of interest are smooth transformations of expansion estimations, the major exception being percentiles).

A Calibrated Estimator for a Total

Suppose we have a calibrated estimator for a total, $t = \sum_S w_j y_j$, where

$$w_j = 1/\pi_j + (\eta^* - \sum_{i\in S^*} [1/\pi_i]\mathbf{x}_i)(\sum_{i\in S^*} [1/\pi_i]\mathbf{x}_i'\mathbf{x}_i)^{-1} [1/\pi_j]\mathbf{x}_j' \quad (6)$$

for $j \in S^*$, and a predetermined value otherwise (chosen so that $w_j \geq 1$ and, perhaps, not too far from $1/\pi_j$), S is the sample, S* a subset containing almost all the elements of S, $\mathbf{x}_i$ is a row vector of covariates whose sum across all elements in the population is η, and $\eta^* = \eta - \sum_{S-S^*} w_i \mathbf{x}_i$. There must also be a vector $\boldsymbol{\lambda}$ such that $\mathbf{x}_j\boldsymbol{\lambda} = \sqrt{(1-\pi_j)}$ for all j (that is to say, either a component of $\mathbf{x}_j$ or a linear combination of components must equal $\sqrt{(1-\pi_j)}$). Since we are dealing with a single-phase sample, (6) is simply equation (2) with $1/\pi_k$ replacing f_k/p_k (i.e., f_k in equation (2) is 1, while p_k is π_k).

To estimate the variance of t, we use equation (1) but replace t with $t^{(v)} = \sum_S w_j^{(v)} y_j$, and $t_{(r)}$ with

$$t_{(r)}^{(v)} = \sum_S w_{j(r)}^{(v)} y_j,$$

where

$$w_j^{(v)} = w_j\sqrt{(1 - 1/w_j)}, \tag{7}$$

and

$$w_{j(r)}^{(v)} = w_j^{(v)}\{1 + (\sum_S w_i^{(v)}\mathbf{x}_i - \sum_{S(r)} w_i^{(v)}\mathbf{x}_i)(\sum_{S(r)} w_i^{(v)}\mathbf{x}_i'\mathbf{x}_i)^{-1}\mathbf{x}_j'\} \tag{8}$$

when $j \in S_{(r)}$ and 0 otherwise.

Observe that $w_j^{(v)} \approx w_j\sqrt{(1-\pi_j)}$, so that $w_j^{(v)} \approx w_j$ when the selection probability for element j is ignorably small. When all element selection probabilities are very small, there is little difference between this delete-a-group jackknife for a total estimator with finite population correction, $v_{J(fpcT)}$, and the standard delete-a-group jackknife, v_J. Moreover, the rather odd assumption that there exists a $\boldsymbol{\lambda}$ such that $\mathbf{x}_j\boldsymbol{\lambda} = \sqrt{(1 - \pi_j)}$ becomes close to the more standard assumption that either a component of $\mathbf{x}_j$ or a linear combination of components is a constant (i.e., $\mathbf{x}_j\boldsymbol{\lambda} = 1$ for some $\boldsymbol{\lambda}$).

In fact, if we were to ignore finite population correction (which we can do for most surveys, but not VCUS), we could estimate the variance of t with equation (1), replacing equation (8) with

$$w_{j(r)} = w_j\{1 + (\sum_S w_i\mathbf{x}_i - \sum_{S(r)} w_i\mathbf{x}_i)(\sum_{S(r)} w_i\mathbf{x}_i'\mathbf{x}_i)^{-1}\mathbf{x}_j'\} \tag{8'}$$

when $j \in S_{(r)}$ and 0 otherwise as long as $\mathbf{x}_j\boldsymbol{\lambda} = 1$ for some $\boldsymbol{\lambda}$. This is what we did for the 1997 Minnesota pilot QAS (see Bailey and Kott 1977).

An Estimator for a Ratio

Suppose t_R is an estimator for a ratio of the form, $t_R = \sum_S w_j y_j / \sum_S w_j z_j$, where w_j is calibrated as above. One can estimate the variance of t with

$$v_{J(fpcR)} = (\sum_S w_j^{(v)} z_j / \sum_S w_j z_j)^2 (14/15)\sum^{15} (t_{R(r)}^{(v)} - t_R^{(v)})^2, \tag{9}$$

where $t_R^{(v)} = \sum_S w_j^{(v)} y_j / \sum_S w_j^{(v)} z_j$, and

$$t_{R(r)}^{(v)} = \sum_S w_{j(r)}^{(v)} y_j / \sum_S w_{j(r)}^{(v)} z_j.$$

This assumes $\mathbf{x}_j\boldsymbol{\lambda} = \sqrt{(1 - \pi_j)}$ for some $\boldsymbol{\lambda}$. Even without this assumption holding, in fact, even without calibration, $v_{J(fpcR)}$ will likely be a reasonable variance estimator; as we shall see.

Alternatively, we could estimate the variance of t_R ignoring finite population correction with equation (1). We need not assume that $\mathbf{x}_j\boldsymbol{\lambda} = 1$ for some $\boldsymbol{\lambda}$. *In fact, the w_i need not even be calibrated in this case* (to see why, observe that multiplying all the weights in t_R by a fixed constant so that $\sum_S w_j$ equals the population size has no effect on the estimator; consequently, all ratio estimators are effectively calibrated on $x_j = 1$).

APPENDIX
Justifying the Delete-a-Group Jackknife Under a Single-Phase, Stratified Sampling Design

Suppose we have a probability sample design with H strata and n_h sampled units within each stratum h. Let us assume that the sample was selected without replacement but the selection probabilities are all so small, and the joint selection probabilities are such, that using the with-replacement variance estimator is appropriate (this rules out systematic sampling from a purposefully-ordered lists). In particular, let us assume that the estimator itself can be written in the form:

$$t = \sum_{h=1}^{H} \sum_{j=1}^{n_h} t_{hj}.$$

Let $q_{hj} = t_{hj} - \sum_g t_{hg}/n_h$. The randomization variance of t is $\text{Var}(t) = \sum^H \text{Var}(\sum t_{h+})$, where $t_{h+} = \sum_j t_{hj}$. Now $\text{Var}(t_{h+})$ can be estimated in a (nearly) unbiased fashion by

$$\text{var}(t_{h+}) = (n_h/[n_h - 1]) \sum_{j=1}^{n_h} q_{hj}^2$$

("nearly" because we are ignoring finite population correction).

In order to estimate Var(t) with a delete-a-group jackknife as suggested in the text, we first order the strata in some fashion and then order the units within each stratum randomly. The sample is partitioned into R (i.e., 15) systematic samples using the resulting ordered list. Let S_r denote one such systematic sample, S_{hr} the set of n_{hr} units in both S_r and stratum h, and $S_{h(r)}$ the set of $n_{h(r)}$ units in stratum h and *not* in r.

The jackknife replicate estimator $t_{(r)}$ is

$$t_{(r)} = \sum_{h=1}^{H} (n_h / n_{h(r)}) \sum_{j \in S_{h(r)}} t_{hj}.$$

Now

$$t_{(r)} - t = \sum_{h=1}^{H} [(n_h / n_{h(r)}) \sum_{j \in S_{h(r)}} t_{hj} - t_{h+}].$$

Treating each $S_{h(r)}$ as a simple random subsample of the sample in stratum h, we have

$$E_2[(t_{(r)} - t)^2] = \sum^{H} Var_2([n_h / n_{h(r)}] \sum_{j \in S_{h(r)}} t_{hj})$$

$$= \sum^{H} (n_h^2/n_{h(r)})[1 - (n_{h(r)}/n_h)] \sum^{n_h} q_{hj}^2/(n_h - 1)$$

$$= \sum (n_h/[n_h - 1])(n_{hr}/n_{h(r)}) \sum q_{hj}^2$$

$$= \sum^{H} (n_{hr}/n_{h(r)}) \, var(t_{h+}),$$

where E_2 denotes expectation with respect to the subsampling.

Observe that for strata where $n_h < R$, $n_{hr}/n_{h(r)}$ is either zero because there are no units in both r and h or $n_{hr}/n_{h(r)}$ is $1/(n_h - 1)$ because there is one unit in both r and h. Since the latter situation occurs in exactly n_h replicates, $\sum^{R} n_{hr}/n_{h(r)} = n_h/(n_h - 1)$.

For strata where $n_h \geq R$, $n_{hr}/n_{h(r)} = O(1/R)$ and $\sum^{R} n_{hr}/n_{h(r)} \approx 1 + O(1/R)$. (Technical note: $z = O(1/R)$ means $\lim_{R \to \infty} R|z|$ is a constant). In fact, when n_h/R is an integer, $n_{hr}/n_{h(r)}$ exactly equals $1/(R - 1)$, and $\sum^{R} n_{hr}/n_{h(r)} = R/[R - 1]$.

Since Var(t) can itself be estimated in an approximately unbiased fashion by

$$var(t) = \sum^{H} (n_h/[n_h - 1]) \sum_j q_{hj}^2,$$

it is not difficult to see that the delete-a-group jackknife variance estimator,

$$v_J = ([R - 1]/R) \sum^{R} (t_{(r)} - t)^2$$

is approximately unbiased for var(t) and thus for Var(t) when all strata are such that $n_h \geq R$ and is biased upward otherwise. Moreover, the relative upward bias is bounded by $([R - 1]/R)\min_h \{1/(n_h - 1)\}$.

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